



# Software Focus Area Presentation





# Outline



- Overview of the Software Focus Area
- Recent Activities
  - EMMC International Workshop 2021
  - Model Development & Software Survey 2021
  - Webinars
- Task Groups



# Software Focus Area



The main purpose of this Focus Area is on motivating, facilitating, and promoting the transfer of software for computational materials science into ready-to-use tools for industry, and on providing a forum especially for industrial end users to express their evolving requirements for materials modelling software.

Details: <https://emmc.eu/focus-areas/software/>



# Software Focus Area: Objectives



- Materials science (materials and materials properties)
- Methodologies and algorithms
- Integrability and interoperability, multiscale modelling
- Ownership, licensing, and legal issues
- Verification and validation
- Distribution, documentation, and training
- Maintenance and support
- Models for sustainable software ecosystems



# Members (May 16, 2021)



- Members: 28
  - University: 6
  - Research Institutes: 9
  - Industry: 13
- Countries: Austria, Belgium, Denmark, France, Germany, Greece, Italy, Poland, Romania, Spain, Switzerland, UK



# EMMC International Workshop 2021



Plenary Speaker: **Nicola Marzari, EPFL**

Session 1: Industrial Requirements  
to Materials Modelling Software

Session 2: From Materials Science  
Software to Industrial Tools



## Speakers

- Kurt Stokbro, Stokbro Invest
- Sophie Loehle, TOTAL
- Jonathan Mueller, VW

## Speakers

- Scott M. Woodley, UCL
- Flavio Souza, Siemens DI SW
- Ellad Tadmor, UMN



# Survey 2020/2021 – Conclusions



- Materials digitalization relies on physics-based modelling approaches, data-driven approaches, and their combination, to accurately predict and optimize industrial products
- The materials research community and software owners provide cutting edge materials modelling software (as FOSS or commercial software, respectively)
- The EMMC focus areas Model Development and Software lead the EMMC activities in their domains and the key researchers' needs are:
  - Software: more accurate, robust, well-documented and validated/verified software, with better availability of parameters data (easy generation of input), applicability (general purpose/demonstrators), scalable performance & lower complexity to use
  - Models: improved capability, accessibility and performance of methods, with better applicability (general purpose over specificity)



# Webinar by Dr. Jonathan Mueller, VW



## Webinar on Advancing Automotive Innovation with Materials Modeling / April 29, 2021 / 16:00 CEST

Home | Events | EMMC ASBL Organisational Member MATERIALS DESIGN presents this webinar by Dr. Jonathan Mueller, Volkswagen AG

### EMMC ASBL Organisational Member MATERIALS DESIGN presents this webinar by Dr. Jonathan Mueller, Volkswagen AG

Date: 29.04.2021 - 29.04.2021

Organisers: EMMC ASBL & OM Materials Design

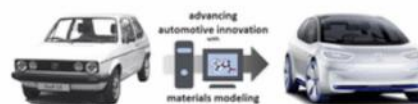
Venue: Webinar / Online

Materials Design, France, an Organisational Member of EMMC ASBL, presents a

#### Webinar on Advancing Automotive Innovation with Materials Modeling

by Dr. Jonathan Mueller, Volkswagen AG

Thursday, April 29, 2021 10 AM EDT / 7:00 AM PDT / 15:00 BST / 16:00 CEST







# Task Groups



1. Success Stories
2. Best Practices for Software Development
3. From Software to Industrial Tools
4. Documentation, Training, and Support
5. Business Models and Sustainability

Example:

## TG 4.2 - Best Practices for Software Development

### Objective

Provide guidelines for Software Development in Materials Modelling

### Related documents

 <b>WEBINAR</b>  Best Practices for Software Development by Volker Eyert (MDS, FR) Kurt Stokbro (Synopsys, DK) EMMC CSA Webinar, recording	 <b>WEBINAR</b>  Introduction to Standards in Software Development for Beginner by Alexandra Simperler (Goldbeck Consulting Ltd., UK) EMMC CSA Webinar, recording	
 <b>WHITE PAPER</b>  White Paper for Standards of Modelling Software Development by Volker Eyert (MDS, FR) Kurt Stokbro (Synopsys, DK) EMMC CSA White Paper	 <b>REPORT</b>  Open Source, free Software and Commercially Supported Software for Materials Modelling by V. Eyert, E. Wimmer (MDS, FR) K. Stokbro (Synopsys, DK) EMMC CSA Expert Group Meeting, report	 <b>DOCUMENTATION</b>  Training Material for Standards in Software Development and where to find it by K. Stokbro (Synopsys, DK) G. Goldbeck, A. Simperler (Goldbeck Consulting, UK) V. Eyert, E. Wimmer (MDS, FR) EMMC CSA Documentation, report

<https://emmc.eu/focus-areas/software/tg-4-2/>



# Task Group 1: Success Stories



- Objective: Demonstrate added value of MM in Industry and Society
- Actions
  - Collect success stories from across the EMMC (members, speakers, ...)
  - Propose/agree on requirements (papers, reports, no theses)
  - Publish online on EMMC website (EMMC internal)
- People: Umberto Martinez, Volker Eyert
- see: <https://emmc.eu/focus-areas/software/task-group-1/>



# Task Group 2: Best Practices for Software Development



- Objective: Provide guidelines for Software Development in MM
- Actions
  - Collect and make available information about best practices for MM software
  - Collect experiences (attention points, application, solver, data management, GUI, multiscale, cloud, FOSS and commercial, ...?)
- People: Volker Eyert, NN

 **WEBINAR** 

Best Practices for Software Development  
by Volker Eyert (MDS, FR)  
Kurt Stokbro (Synopsys, DK)

EMMC-CSA Webinar, recording

 **WEBINAR** 

Introduction to Standards in Software Development for Beginner  
by Alexandra Simperler (Goldbeck Consulting Ltd., UK)

EMMC-CSA Webinar, recording

 **WHITE PAPER** 



White Paper for Standards of Modelling Software Development  
by Volker Eyert (MDS, FR)  
Kurt Stokbro (Synopsys, DK)

EMMC-CSA White Paper

 **REPORT** 

Open Source, free Software and Commercially Supported Software for Materials Modelling  
by V. Eyert, E. Wimmer (MDS, FR)  
K. Stokbro (Synopsys, DK)

EMMC-CSA Expert Group Meeting, report

 **DOCUMENTATION** 

Training Material for Standards in Software Development and where to find it  
by K. Stokbro (Synopsys, DK)  
G. Goldbeck, A. Simperler (Goldbeck Consulting, UK)  
V. Eyert, E. Wimmer (MDS, FR)

EMMC-CSA Documentation, report



# Task Group 3: From Software to Industrial Tools



- Objective: Encourage professionalization of MM software
- Actions
  - Identify requirements for transforming MM software into industrial tools
  - Identify software, which has successfully completed transition from academia to industry-readiness
  - Contact and learn from companies, which successfully completed such transformation processes (Siemens DI SW, Global TCAD Solutions, Synopsys, VASP GmbH, Materials Design, ...)
- People: NN

EMMC PRESENTATION

Building a Materials Engineering Software Product: From Academic Research to Commercialization

by Flavio Souza  
(Siemens Digital Industries Software, US)

EMMC2021 / Session 8, recording

EMMC PRESENTATION

Development and Evolution of Materials Modelling Software

by Scott Woodley (UCL, UK)

EMMC2021 / Session 8, recording

EMMC PRESENTATION

Addressing Industrial Needs for Atomistic Simulations through OpenKIM

by Ellad Tadmor (University of Minnesota, US)

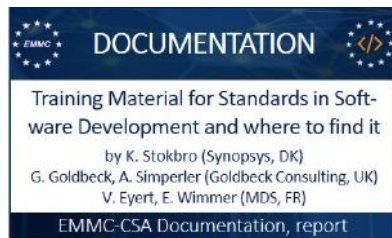
EMMC2021 / Session 8, recording



# Task Group 4: Documentation, Training, and Support



- Objective: Provide links to industry-level training material
- Actions
  - Survey to collect experiences with software documentation, training and support, as well as needs for improvements
  - Look at: in-house coding, FOSS, commercial software, ... ?
  - Achieve customer success
- People: NN





# Task Group 5: Business Models and Sustainability



- Objective: Identify business models in industrial software deployment
- Actions
  - Collect information from earlier studies in EMMC
  - Circulate some questions to software partners, ask for input from previous EC project participations in Materials Software area
- People: Stijn Donders, Alexandra Simperler

**REPORT**

Sustainable economic framework for materials modelling software

by G. Goldbeck, A. Simperler (Goldbeck Consulting, UK)

EMMC-CSA Expert Group Meeting, report

**WEBINAR**

How to find the right business model for materials modelling software

A. Simperler, G. Goldbeck (Goldbeck Consulting, UK)  
N. Konchakova, D. Höche (Hereon, DE)

EMMC-CSA Webinar, recording

**WORKSHOP**

Business Models for Materials Modelling

hosted by  
A. Simperler, G. Goldbeck (Goldbeck Consulting, UK)  
N. Konchakova (Hereon, DE)

EMMC-CSA Workshop, recording

**WHITE PAPER**

Business Models and Sustainability for Materials Modelling Software

by G. Goldbeck, A. Simperler (Goldbeck Consulting, UK)

EMMC-CSA White Paper

**PRESENTATION**

Business opportunities for materials science software

by Kurt Stokbro (Stokbro Invest, DK)

EMMC2021 / Session 6, recording

**PRESENTATION**

Building a Materials Engineering Software Product: From Academic Research to Commercialization

by Flavio Souza (Siemens Digital Industries Software, US)

EMMC2021 / Session 8, recording



# Thank you!

